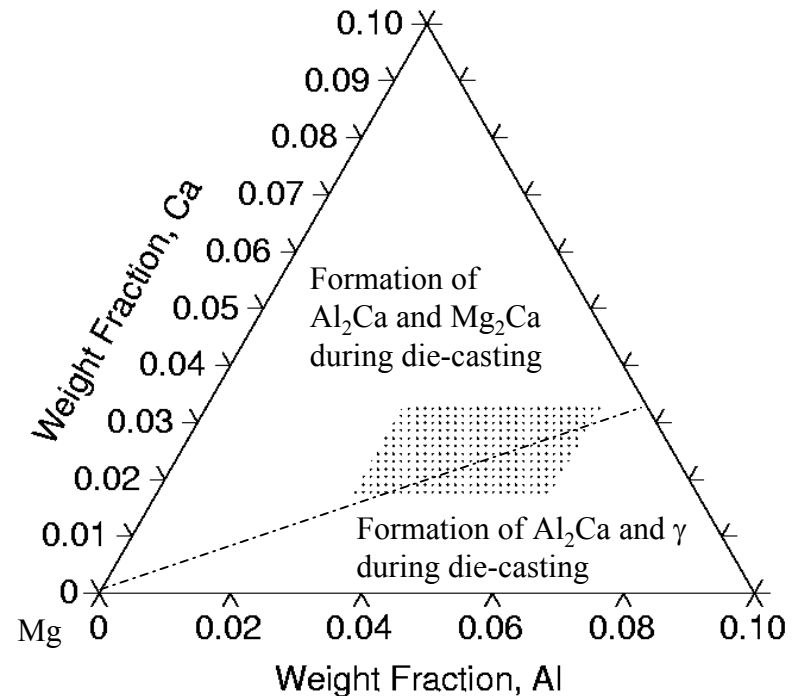


CAREER: Integrated Teaching and Research Activities on Computational Thermodynamics and System Materials Design of Magnesium Alloys

Zi-Kui Liu, The Pennsylvania State University, **DMR-9983532**

Magnesium is the eighth most abundant element in the Earth's crust. It is the lightest structural material with a density of 1.741 g/cm^3 , in comparison with the densities of Al (2.70 g/cm^3) and Fe (7.86 g/cm^3). This makes magnesium alloys particularly attractive for transportation applications such as automobiles and helicopters for weight reduction and higher fuel efficiency. Computational thermodynamics indicates that key issue in improving the creep property of Mg-Al-Ca alloys is to control the Al:Ca ratio as shown in the left diagram.



New composition designation for the Mg-Al-Ca system.

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Education: Six undergraduate students (two female and one black) did their BS thesis with the PI on various computational projects. One of them, Melissa Marshall, received 2001 Xerox Award for B.S. thesis. Two seniors are currently working on their BS theses with the PI. Two American students finished their MS theses in the PI's lab, and one international student finished the PhD thesis and is presently teaching in Turkey.

Outreach: PI organized workshops in summer 2001 and 2002 with participants from academy and industry. The following is a photo taking from 2001 workshop with PI assisting participants.



The computer facility was established by the project **DMR-0073836**.